trans-2-Ethyl-3-methylthiophane

Other names:	2-Ethyl-3-methyltetrahydrothiophene, trans- trans-2-Ethyl-3-methyl-thiacyclopentane
Inchi:	InChI=1S/C7H14S/c1-3-7-6(2)4-5-8-7/h6-7H,3-5H2,1-2H3/t6-,7+/m0/s1
InchiKey:	XNZCGHZDGZDSBU-NKWVEPMBSA-N
Formula:	C7H14S
SMILES:	CCC1SCCC1C
Mol. weight [g/mol]:	130.25
CAS:	61568-36-3

Physical Properties

Property code	Value	Unit	Source
gf	76.76	kJ/mol	Joback Method
hf	-102.41	kJ/mol	Joback Method
hfus	12.55	kJ/mol	Joback Method
hvap	36.94	kJ/mol	Joback Method
log10ws	-2.40		Crippen Method
logp	2.538		Crippen Method
mcvol	114.980	ml/mol	McGowan Method
pc	3269.04	kPa	Joback Method
rinpol	986.00		NIST Webbook
rinpol	986.00		NIST Webbook
tb	418.00	K	Joback Method
tc	628.19	K	Joback Method
tf	258.76	K	Joback Method
vc	0.413	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	221.88	J/mol×K	418.00	Joback Method
cpg	237.68	J/mol×K	453.03	Joback Method
cpg	252.69	J/mol×K	488.06	Joback Method
cpg	266.93	J/mol×K	523.09	Joback Method
cpg	280.42	J/mol×K	558.12	Joback Method

cpg	293.20	J/mol×K	593.16	Joback Method
cpg	305.28	J/mol×K	628.19	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C61568363&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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